Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.89e-10 mmHg

Global applicability domain: Outside

Local applicability domain index: 2.83e-01

Confidence level: 2.93e-01

Nearest Neighbors from the Training Set

Image not found
Isophorone diamine
Measured: 4.00e-14
Predicted: 1.87e-02

Image not found
Tetrachlorovinphos
Measured: 3.00e-09
Predicted: 9.39e-07

Image not found
Z-Tetrachlorvinphos
Measured: 3.00e-09
Predicted: 9.39e-07

Image not found
Pyridaphenthion
Measured: 4.00e-12
Predicted: 1.35e-07

Image not found
Sevoflurane
Measured: 2.48e-08
Predicted: 264

Image not found
Halfenprox
Measured: 1.35e-06
Predicted: 7.31e-09